

Theoretical study of the reaction of S^+ with vibrationally excited H_2

A. Zanchet¹, O. Roncero², A. Aguado³ and M. Agúndez⁴

¹*Instituto de Estructura de la materia, C.S.I.C., Serrano 123, 28006 Madrid, España.*

²*Instituto de Física Fundamental, C.S.I.C., Serrano 123, 28006 Madrid, España.*

³*Departamento de Química Física, Facultad de Ciencias C-XIV,
Universidad Autónoma de Madrid, 28049 Madrid, España.*

⁴*Laboratoire d'Astrophysique de Bordeaux, Observatoire Aquitain des Sciences de l'Univers,
Université Bordeaux 1, 2 rue de l'Observatoire, BP 89, 33271 FLOIRAC CEDEX, France.*

E-mail: zanchet@iem.cfmac.csic.es

The SH^+ molecule has been recently observed in interstellar medium, although its mechanism of formation is still not clear. One of the possible reaction leading to this molecule is the collision of the sulfur ion with H_2 , the most abundant molecule in interstellar medium. The reaction $S^+ + H_2 \rightarrow SH^+ + H$ is endothermic by 0.86 eV and, therefore, is expected to have small rate constant at low temperature. Nevertheless, recent studies indicate that vibrationally excited H_2 , which can be encountered in dense photon dominated regions, may favour this reaction and make it the main source of SH^+ in such interstellar regions [1].

In this work, we will present the reaction dynamics study of the title reaction, taking in account the vibrational excitation of the H_2 molecule. The calculations were done using quantum and quasi-classical dynamics methods using an accurate potential energy surface we built based on *ab initio* electronic structure calculations. The cross sections and rate constants were calculated for several vibrational level of H_2 to check the effect of vibration of H_2 and how it enhance the reactivity of this system.

[1] M. Agúndez et al., Ap. J. **713**, 662 (2010).